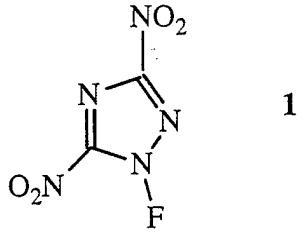


## REPORT DOCUMENTATION PAGE

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<p>The predicted heat of formation and impact sensitivity of the recently-synthesized dinitro-N-fluorotriazole <b>1</b>,</p> <div style="text-align: center;">  <p style="text-align: center;"><b>1</b></p> </div> <p>based on computational analyses, are:</p> $\Delta H_f(\text{gaseous}) = 77 \text{ kcal/mole} = 435 \text{ cal/gram}$ $\Delta H_f(\text{solid}) = 56 \text{ kcal/mole} = 316 \text{ cal/gram}$ $h_{50} = 126 \text{ cm}$			
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Dr. Richard S. Miller

Technical Report No. 90

COMPUTED HEAT OF FORMATION AND IMPACT SENSITIVITY  
OF A NEW DINITRO-N-FLUOROTRIAZOLE

by

Peter Politzer, J. S. Murray and M. E. Grice

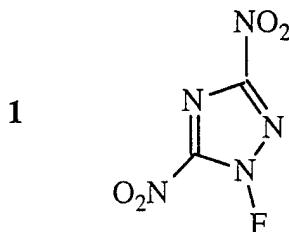
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New Orleans, LA 70148

March 7, 1996

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The dinitro-N-fluorotriazole **1** has recently been synthesized [1] and characterized crystallographically [2].



We now report our computed heat of formation and impact sensitivity for **1**.

The gas phase heat of formation was calculated using our density functional procedure [3]. It was converted to the solid phase value by means of eq. (1),

$$\Delta H_f(\text{solid}) = \Delta H_f(\text{gaseous}) - \Delta H_{\text{sub}} \quad (1)$$

in which  $\Delta H_{\text{sub}}$  is the heat of sublimation.  $\Delta H_{\text{sub}}$  and the impact sensitivity,  $h_{50}$ , were obtained by means of correlations that we have developed between these properties and computed quantities related to electrostatic potentials on molecular surfaces [4,5]. The latter were calculated at the *ab initio* HF/STO-5G//HF/3-21G level.

The results follow:

$$\Delta H_f(\text{gaseous}) = 77 \text{ kcal/mole} = 435 \text{ cal/gram}$$

$$\Delta H_f(\text{solid}) = 56 \text{ kcal/mole} = 316 \text{ cal/gram}$$

$$h_{50} = 126 \text{ cm}$$

## References

- [1] R. J. Schmitt, SRI International.
- [2] R. Gilardi, Naval Research Laboratory.
- [3] D. Habibollahzadeh, M. E. Grice, M. C. Concha, J. S. Murray and Peter Politzer, *J. Comp. Chem.* 16, 654 (1995).
- [4]  $\Delta H_{\text{sub}}$ : E. DeSalvo, E. Miller, J. S. Murray and P. Politzer, unpublished work.
- [5]  $h_{50}$ : J. S. Murray, P. Lane and P. Politzer, *Mol. Phys.* 85, 1 (1995).